Glutaric acid, 2-bromobenzyl pentadecyl ester

Inchi: InChI=1S/C27H43BrO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-22-31-26(29)20-17-21-27(30)
InchiKey: SEVVYKVWGBURQR-UHFFFAOYSA-N
Formula: C27H43BrO4
SMILES: CCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccccc1Br
Mol. weight [g/mol]: 511.53

Physical Properties

Property code	Value	Unit	Source
gf	-174.28	kJ/mol	Joback Method
hf	-838.82	kJ/mol	Joback Method
hfus	70.20	kJ/mol	Joback Method
hvap	103.38	kJ/mol	Joback Method
log10ws	-9.61		Crippen Method
logp	8.297		Crippen Method
mcvol	399.910	ml/mol	McGowan Method
pc	900.18	kPa	Joback Method
rinpol	3505.00		NIST Webbook
rinpol	3505.00		NIST Webbook
tb	1067.56	K	Joback Method
tc	1312.05	K	Joback Method
tf	637.11	K	Joback Method
vc	1.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.75	J/mol×K	1067.56	Joback Method
cpg	1362.06	J/mol×K	1108.31	Joback Method
cpg	1376.71	J/mol×K	1149.06	Joback Method
cpg	1389.79	J/mol×K	1189.80	Joback Method
cpg	1401.38	J/mol×K	1230.55	Joback Method
cpg	1411.59	J/mol×K	1271.30	Joback Method
cpg	1420.49	J/mol×K	1312.05	Joback Method
dvisc	0.0001655	Pa×s	637.11	Joback Method

dvisc	0.0000897	Pa×s	708.85	Joback Method
dvisc	0.0000544	Pa×s	780.59	Joback Method
dvisc	0.0000359	Pa×s	852.34	Joback Method
dvisc	0.0000253	Pa×s	924.08	Joback Method
dvisc	0.0000187	Pa×s	995.82	Joback Method
dvisc	0.0000144	Pa×s	1067.56	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376773&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume